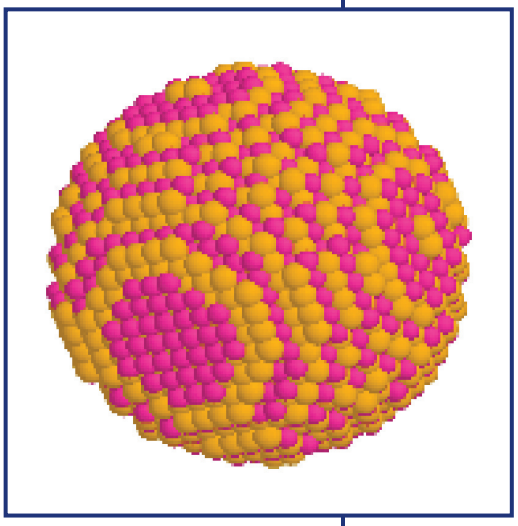
Smaller is Better

Nanoparticle simulation achieves sustained performance of over 81% of theoretical peak performance on Cray XT3



Nanoparticles represent high-density storage solutions.

Materials

Materials are the foundation of technological advancement, from stone, to bronze, to iron, to steel. Today their revolutionary impact on technology is seen in plastics, semiconductors, superconductors, super alloys, and, in the future, nanostructured materials. To that end we are now witnessing the merger of materials science—macroscopic properties of matter – and condensed matter physics—microscopic behavior. Calculations performed at the electronic level are poised to accurately describe macroscopic measurements using high-performance computing. Computing power, such as that in Oak Ridge National Laboratory's National Leadership Computing Facility (NCLF), and algorithm design requirements underlie the need for steady advances in both to successfully model new materials.

Store Data with the Flip of a Spin

High-density data storage relies on the ability to alter the magnetic state of a material. Large or "bulk" materials composed of FePt have exceptionally high magnetocrystalline anisotropy energy (MAE); essentially, once the magnetic state has been altered in FePt, it would require a great deal of energy to reverse it. Thus, any change to the magnetic state of FePt is effectively permanent. Conversely, materials with low MAE have a much smaller barrier to magnetic state changes; temperature increases can cause random scrambling of previously set magnetic states.

Great excitement has arisen over the development of processes to create nanoparticles of uniform size. By engineering their size, shape and surface chemistry, the capacity for information storage can be increased dramatically in comparison with bulk materials. Major outstanding problems include designing the nanoparticles to obtain high MAE. The MAE is proportional to the volume of the particle (smaller particle, smaller MAE). Modeling can help unravel the relationship between chemical, structural, and magnetic properties of these promising information storage materials.

Future of Data Storage

In a seminal paper, Weller and his group [Sun et al. *Science* 287, 1989 (2000)] have shown that it is possible to synthesize large numbers of nanometer-sized FePt particles with uniform size and with effective magnetic anisotropy sufficiently large to be used for magnetic storage media that can accommodate tens of terabits per square inch storage density. The magnetization at room temperature would be stable, and magnetically stored information in a single particle could be retained for the lifetime of the storage medium. With this breakthrough, one of the key roadblocks to ultra-high-density disc drives was removed, but a new one was created: Since the particle's volume is now only a few nanometers cubed, the magnetization cannot be reversed with conventional writing techniques. In other words, although information can be stored, it cannot be written!

A large effort is currently under way to find new ways to write magnetic bits, that is, how the magnetic moment in these nanoparticles can be switched deliberately with a nanometer-sized write head at rates appropriate for use in hard drives. One of the major scientific challenges is that, despite their small size, these nanoparticles are complex. However, complexity can in this case be used to devise a new switching mechanism, provided the magnetic properties in these particles can be understood at the atomic scale.

The modeling method used for these microscopic studies is unique in two ways. First, the underlying electronic structure code (LSMS) is the only one that is presently capable of performing the necessary, fully relativistic all electron calculations for magnetic systems with several thousand atoms. Secondly, the systems will be simulated under non-zero temperature conditions.

Temperature fluctuations will alter magnetic responses of materials; for materials with small MAE, slight increases in the temperature could "wipe" out the data stored, as the magnetic state of the internal particles fluctuates, too. Historically, first principles modeling of magnetic states of materials has been limited to studies at zero temperature. For a more realistic understanding of the interplay between materials, magnetic states, and fluctuations, complex calculations are required that include finite-temperature effects. For this, we will use a recently developed extension of the Wang-Landau algorithm suitable to calculate joint densities of states and hence entropy as well as the free energy of magnetic nanostructures.

The Need for Speed

The Wang-Landau algorithm relies on multiple random walkers that communicate small amounts of data after each step; it is an inherently parallel method. The key to the success of first-principles Wang-Landau is the ability to rapidly perform the magnetic energy evaluations for nanoparticles containing thousands of atoms. This requires linear scaling codes, efficient numerical methods, and fast communication between processors. This is achieved by the LSMS running on the NCCS Cray XT3, as demonstrated by the achievement of over 81% of theoretical peak performance for the non-collinear magnetic structure of particles containing up to 2662 atoms. With this type of optimized algorithmic and computing performance, a realistic thermodynamic description of the magnetic behavior of FePt nanoparticles is anticipated in the near future. Thus far the LSMS has shown variation in moment size and orientation as a function of position within a nanoparticle and with nanoparticle size and composition.